

Correlation Functions from Quantum Cluster Algorithms: Application to $U(1)$ Quantum Spin and Quantum Link Models *

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We demonstrate how correlation functions for non-diagonal operators can be measured with the loop-cluster algorithm for quantum spin models. We introduce the $U(1)$ quantum link model and present the construction of a cluster algorithm for the model. We further show how an improved estimator for Wilson loops can be realized with the flux-cluster algorithm.

1. INTRODUCTION

Cluster algorithms have been established as very efficient tools for the numerical simulation of both classical and quantum spin systems. In particular, for quantum spin systems, the loop-cluster algorithm [1] has allowed very efficient studies of the 2-d Heisenberg antiferromagnet utilizing a continuous Euclidean time formulation [2]. An interesting development is the observation [3] that non-diagonal correlation functions can be measured with the loop-cluster algorithm. The methodology is carried over to the numerical study of the $U(1)$ quantum link model (QLM) which is a new, discrete formulation of Wilson's gauge theory [4]. A flux-cluster algorithm has been constructed and an improved estimator for Wilson loops is shown to exist.

2. THE LOOP-CLUSTER ALGORITHM

Consider the 2-d quantum XY model, defined by the Hamiltonian

$$H = -J \sum_{x,\mu=1,2} [S_x^1 S_{x+\hat{\mu}}^1 + S_x^2 S_{x+\hat{\mu}}^2], \quad (1)$$

which couples nearest-neighbor quantum spin operators \vec{S}_x . The quantum partition function

$$Z = \text{Tr} \exp(-\beta H) \quad (2)$$

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is formulated as a (2+1)-d path integral with the system evolving in Euclidean time with extent β . Time is discretized in small steps of size ϵ and the Hamiltonian is decomposed in an even-odd pattern [2] such that the transfer matrix between two subsequent time slices is a product of mutually commuting elementary transfer matrices

$$\mathcal{T} = \exp(\epsilon J [S_x^1 S_{x+\hat{\mu}}^1 + S_x^2 S_{x+\hat{\mu}}^2]). \quad (3)$$

A complete set of states is inserted in each time-slice to form the path integral. For $s=1/2$ spins, the 4×4 matrix elements of \mathcal{T} between the eigenstates — for example in the S^3 basis — of the two spins, define the Boltzmann weights for the interaction between two pairs of spin states in adjacent time slices. The loop-cluster algorithm starts on a random spin state and examines the weight of the interacting quartette of spins. It joins probabilistically the spin to one of the other spins and the process continues until a loop of spin states is formed. The loop is the worldline of evolution of a spin state in the (2+1)-d periodic volume. The cluster rules are ergodic and obey detailed balance. The spin states in the cluster are then flipped resulting in a very efficient update of the system. It is shown in [3] that the quantum partition function is mapped to a quantum random cluster model similarly to the Fortuin-Kasteleyn mapping for the Potts model. The mapping holds at the operator level and therefore the loop-cluster has geometrical properties independent of the chosen basis. Due to the discrete-

ness of the Hilbert space, the continuum limit $\epsilon \rightarrow 0$ can be taken and the algorithm can be implemented in the continuum of the Euclidean time direction [2].

The expectation value of a Green's function like

$$\langle S_x^1 S_y^1 \rangle = \frac{1}{Z} \text{Tr}[S_x^1 S_y^1 \exp(-\beta H)] , \quad (4)$$

appears impossible to measure from the ensemble of configurations that contribute to Z . This is because the insertion of the non-diagonal operator S^1 creates a configuration that never contributes to the partition function. The important observation made in [3] is that the loop-cluster algorithm generates configurations that can be thought as contributing to (4) also. Indeed, consider the loop which passes from the sites x and y on a fixed time-slice. We can imagine that we cut the loop on this time-slice and flip only half of the cluster. Since S^1 flips the S^3 eigenstates, this process precisely contributes to (4). We therefore generate the loops with the algorithm and then perform cuts on all time-slices which dissect the loop in two pieces. If each half can be flipped independently, a +1 contribution is registered for the correlation function between the cutting sites. In this way, an *improved estimator* for the non-diagonal Green's function (4) has been realized which does not suffer from any sign cancelations.

3. THE $U(1)$ QUANTUM LINK MODEL

A new formulation for lattice gauge theories has been proposed in [4]. Here we study the pure $U(1)$ gauge theory on the lattice. We consider the quantization of the links, i.e. the promotion of the classical link field $u_{x,\mu} = \exp(i\varphi_{x,\mu})$ to a quantum link operator $U_{x,\mu}$ acting on the link-based Hilbert space. The $U(1)$ QLM is defined through the 4-d Hamiltonian

$$H = -J \sum_{x,\mu \neq \nu} [U_{x,\mu} U_{x+\hat{\mu},\nu} U_{x+\hat{\nu},\mu}^\dagger U_{x,\nu}^\dagger] \quad (5)$$

which is invariant under the local $U(1)$ transformations at the left and right ends of the link

$$\begin{aligned} U'_{x,\mu} &= \prod_y \exp(i\alpha_y G_y) U_{x,\mu} \prod_z \exp(-i\alpha_z G_z) \\ &= \exp(i\alpha_x) U_{x,\mu} \exp(-i\alpha_{x+\hat{\mu}}) . \end{aligned} \quad (6)$$

The transformation law results in the following commutation relations between the local generator of the symmetry G_x and the link operators

$$[G_y, U_{x,\mu}] = (\delta_{y,x} - \delta_{y,x+\hat{\mu}}) U_{x,\mu} . \quad (7)$$

These relations are satisfied if we represent the link operators and the $U(1)$ generator as

$$\begin{aligned} U_{x,\mu} &= S_{x,\mu}^1 + iS_{x,\mu}^2 = S_{x,\mu}^+ \\ G_x &= \sum_{\mu} (S_{x,\mu}^3 - S_{x-\hat{\mu},\mu}^3) , \end{aligned} \quad (8)$$

where $S_{x,\mu}^a$ is a spin operator associated with a link, with the usual commutation relations

$$[S_{x,\mu}^a, S_{y,\nu}^b] = i\delta_{xy}\delta_{\mu\nu}\epsilon^{abc}S_{x,\mu}^c . \quad (9)$$

The operator $S_{x,\mu}^3$ represents the electric flux on the link and $U_{x,\mu}$ acts as a flux raising operator. The Hilbert space per link is the space of the local $SU(2)$ algebra representation and it is therefore finite. The quantum partition function

$$Z = \text{Tr} \exp(-\beta H) \quad (10)$$

is formulated as a (4+1)-d path integral with the system evolving in a fifth dimension of extent β . When β exceeds a critical value, the excitations of the model are in the Coulomb phase of the 5-d Abelian gauge theory. Due to the infinite correlation length in the 5-d Coulomb phase, if the extent of the fifth dimension β is finite, the theory will dimensionally reduce to the 4-d Abelian gauge theory. The phase transition of Wilson's $U(1)$ gauge theory can be studied from the growth of the correlation length near the critical fifth dimension extent of the $U(1)$ QLM. Even spin-1/2 quantum links may suffice for the dimensional reduction — more on the phase diagram of the model for general spin in [6].

4. THE FLUX-CLUSTER ALGORITHM

A cluster algorithm has been constructed for the spin-1/2 $U(1)$ QLM [5,7]. The fifth dimension in (10) is discretized in small steps of size ϵ and a complete set of states is inserted at each time-slice. Each plane of the 4-d lattice Hamiltonian is decomposed in a checker board fashion of

even and odd plaquettes. Only one type of plaquettes is allowed to interact between two subsequent time-slices so that the full transfer matrix is a product of commuting transfer matrices

$$\mathcal{T} = \exp(\epsilon J [U_{x,\mu} U_{x+\hat{\mu},\nu} U_{x+\hat{\nu},\mu}^\dagger U_{x,\nu}^\dagger + U_{x,\nu} U_{x+\hat{\nu},\mu} U_{x+\hat{\mu},\nu}^\dagger U_{x,\mu}^\dagger]) . \quad (11)$$

The 16×16 matrix elements of \mathcal{T} define the Boltzmann weights of the checker boarded cubes carrying the interaction of 8 electric flux states $e_{x,\mu,t}$ in the path integral

$$Z = \prod_{x,\mu,t} \sum_{e_{x,\mu,t}=\pm 1/2} \exp(-S[e]) . \quad (12)$$

The flux-cluster algorithm builds a cluster of links in the 5-d volume and updates the system by flipping the electric flux on the links which belong to the cluster. The cluster starts on a random link and probabilistically assigns some of the 8 links of the interaction cube in the cluster. The cluster rules are ergodic and obey detailed balance. The process continues through the 5-d volume until the cluster is completed. The cluster is a 2-d surface embedded in the 5-d volume and is the worldsheet of the evolution in the fifth dimension of open and closed electric flux strings. Open flux strings are allowed because the Gauss law is not enforced in (10). Due to the discreteness of the flux, the algorithm can operate directly in the continuum limit $\epsilon \rightarrow 0$ of the Euclidean time direction [2,7].

The order parameter for the gauge theory is the expectation value of Wilson loops W_C which is the product of quantum link operators $U_{x,\mu}$ along some closed curve C in the 4-d lattice at a fixed value of t . The link operators on the curve raise the electric flux and therefore the configurations which are generated by the algorithm will never contribute to the expectation value

$$\langle W_C \rangle = \frac{1}{Z} \text{Tr}[W_C \exp(-\beta H)] . \quad (13)$$

The flux-cluster algorithm provides the solution again. Each cluster which is generated and flipped contributes to Z , but it may also contribute to $\langle W_C \rangle$. The operator W_C flips the orientation of the electric flux along the curve C . If

the cluster is cut along C and the flux is flipped on only one of the pieces, a +1 contribution to $\langle W_C \rangle$ is obtained. Notice that if the cluster is connected to itself by wrapping over the periodic fifth dimension, i.e. has the topology of a torus, it cannot be cut in two disjoint pieces along a circle and does not contribute to $\langle W_C \rangle$. With the flux-cluster algorithm therefore, a lot of information can be collected by examining the topology of the cluster and cutting the cluster along fixed time-slices. Each closed curve cut which allows independent flips of the two parts offers a +1 contribution to the corresponding Wilson loop. We have therefore realized an *improved estimator* with no sign cancelations for the order parameter of the Abelian gauge theory.

In conclusion, the quantum link formulation and the cluster algorithm have provided a complete setup for an efficient study of the Abelian lattice gauge theory.

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